# More reference spectroscopic data on the Internet! FTIRsearch Nicolet/Galactic Industries new joint venture

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A new joint venture between Galactic Industries and Nicolet has further added to the list of innovations in reference spectroscopic data delivery. The internet service running under http://ftirsearch.com/ was launched on 17 April 2000. With this new service coming on-line, the spectroscopist must now regard the year 2000 as one of the best for the introduction of new strategies and options for reference database access and service ever!

## The co-operation

This service has been developed in a similar bi-lateral manner to the other internet spectroscopic database service featured earlier in the year with a database supplier—in this case Nicolet—providing the reference data and a well-known spectroscopic data handling company—in this case Galactic Industries Corporation—using their knowledge to provide the software server for the web site. This type of collaboration can only be beneficial for the end-users who have suffered for many years from their service providers always trying to go-it alone and provide all-singing, all-dancing solutions to what is, in computing terms, a small market place. Strategic co-operations with each partner concentrating on their own strengths can only improve the products and services being made available to the spectroscopic users in the long run.

## Installation

Conventional off-the-shelf browser technology is all that is required to use the main spectral search section of the FTIRsearch site. However, a plug-in is required to use a useful spectral interpretation guide. This plug-in called "Neuron" needs to be installed from the company formerly known as Asymetrix Learning Systems available from the http://click2learn.com/ web site. This Toolbook plug-in is for files with .tbk extension and is required for the FT-IR spectral interpretation guide section of the utilities available. If this free utility is not going to be used then the plug-in is not required. The recommended version is Neuron is 6.5 and a direct link is made available on the web site to this version. The latest version of Neuron is 7.2 but this should *NOT* be used. Downloading was not trivial from their web site as they use an FTP server rather than HTTP and this didn't like our firewall system. If you have problems contact Nicolet or Galactic.

Once your system is installed (and you can check over your browser if the plug-in installation has been successful) you can go to the web site at http://ftirsearch.com and obtain an account. Readers who have registered with *Spectroscopy Europe* as using IR or Raman spectroscopy should have received a certificate inserted in their copy with a code number for an account credit on this system. This should be used once you have registered for an account by going to the "member's menu", opting for "redeem credit certificate" and then entering the long certificate number. If nothing has changed between now and going to press the certificate should credit you with 50 credits—enough for two full spectral searches or five text searches.

The account login procedure consists of your registered email address as user name and a password which is assigned to new members upon registration but which can be altered once logged in by going to the members area and updating your registered profile (this is strongly recommended by the service providers!).

Since no special software needs to be installed to use the majority of the service (excluding the FT-IR interpreter), a user is not tied to access from a particular site. The registered user could just as easily check his or her results as well as review previous searches from the local Internet cafe or from home as from their normal workplace.

## The databases

For me probably the most interesting point about testing this system—apart from the aspect of Internet access—was the chance to take a look at one of the reference spectroscopic data collections not normally found in regular use. This is mainly due to the restricted access policy of the database owners to their spectrometer customers. A policy which has been loosened in the past to my knowledge for major chemical companies but not for academic use in general. An overview of the available reference data giving a insight into the diverse origins is provided in Table 1.

As can be seen from Table 1 a number of collections occur twice and this is something which will need to be sorted out by the system developers in future releases. The associated support data for each database also depends on its origin and how much time and trouble was spent by the original database collector. The combination of all text fields into a general text search (see below) seems a good approach considering the differing content. Some databases have CAS naming, others IUPAC and many include "other names" where they have been supplied.

The resolution at which the various collections have been measured varies between databases and also isn't always clear as often "digital resolution" is provided rather than spectral. It is possible (and common) to measure GC/IR data at 8 or 16 cm$^{-1}$ but with a digital resolution of 2 cm$^{-1}$; it is to be

**Table 1. Databases available on FTIRSearch.com.**

| Collection | Size | Resolution (cm$^{-1}$) | Comments |
|---|---|---|---|
| Aldrich FT-IR Collection, Edition II | 18,454 | 2 | |
| Sigma Biochemicals | 10,411 | 2 | |
| Sigma Steroids | 3011 | 2 | |
| Aldrich Vapor Phase | 6611 | 2 | 6543 heated (Aldrich), 68 room temp (Nicolet) |
| EPA Vapor Phase | 3300 | 4 | |
| Hazardous Chemical Vapor Phase | 304 | 2 | |
| Nicolet Vapor Phase | 8654 | 0.5–2 | 6543 Aldrich, 1345 EPA, 622 Uni. Wurzburg, 65 Uni. Hannover, 79 Nicolet |
| TGA Vapor Phase | 460 | 4 | |
| Coatings Technology | 2507 | 2 | |
| Hummel Polymers and Additives | 2011 | 4 | |
| Industrial Coatings | 1961 | 4 | |
| Polymers, Additives and Plasticizers | 1799 | 2 | +1509 polymers, 290 plasticizers |
| Rubber Compounding Materials | 350 | 2 | |
| Aldrich Solvents | 246 | 2 | from only 132 solvents, 127 liquid samples, rest vapour phase! |
| Commercial materials | 90 | 2 | Propylene additives |
| | 48 | 2 | Epoxy resins |
| | 56 | 2 | Painter Mineral (Prof. Painter!) |
| | 18 | 2 | 14 Explosives 4 non– |
| Flavors & Fragrances | 667 | 2 | |
| Food Additives | 519 | 2 | |
| Hazardous Chemical Condensed Phase | 411 | 2 | |
| Inorganic Library | 1803 | 4 | Incl. 600 minerals, 296 boron, 210 commercial, indicators and dyes |
| Lubricants and Oils | 2114 | 4 | 538 ATR, 538 ATR corrected, 1038 transmission |
| Paper Materials | 301 | 2 | |
| Pharmaceutical Excipients | 300 | 2 | |
| Surfactants | 637 | 4 | |
| US Geological Survey Minerals | 78 | 4 | Mostly silicates |
| Georgia State Forensic Drugs | 1940 | 4 | |
| Synthetic Fibers | 376 | 2 | |
| Toronto Forensics | 3549 | 4 | |
| **TOTAL** | **72,986** | | |
| | | | |
| Aldrich Raman | 14,033 | 2 | Nd:YVO$_4$ (1064 nm) laser |
| Pharmaceutical Excipients Raman | 300 | 2 | |
| Polymers by Raman | 99 | 4 | |
| Forensics by Raman | 175 | 4 | |
| Organics by Raman | 1000 | 4 | |
| **TOTAL** | **15,607** | | |

hoped that in future releases the spectral resolution will be added wherever possible. It can of course be regarded as irrelevant as the data has been mathematically de-resolved to a digital resolution of 4 cm$^{-1}$ anyway for database searching but purists will want to know this information. The spectra displayed by the Java applet are at the full resolution of the collection (see Table 1).

# Text searching

The simplest way of looking up data in the database is by means of the text searching options. Calling this a text search is strictly accurate but a bit misleading, as a number of options are available including CAS number searching and molecular formula (see Figure 1).

This is a cheaper option than the full spectral search which will be described below. One advantage of trying out this system from Germany is that during the morning the Americans are asleep and the system is quick. During the afternoon I had originally some teething troubles with incomplete data transfer and display within spectral searching mode. This may well have been due to system problems at my end, since the untimely death of our T1 hardware forced us to resort to an ISDN line for our entire institute! As can be seen from the examples, I have chosen one of the areas we feel particularly weak in—inorganics—as I wished to investigate for our work the strengths of the new database service in this region.

Figure 2 shows that we were successful in the search for lead sulphate using the molecular formula option!

# Spectral searching

Searching the databases by means of full spectrum search is possible through two entry points: one called simple spectral search and the other advanced. The only difference between the two is the reported ability to opt for different search algorithms in the advanced window.

Initially, however, it is necessary to upload your unknown spectrum onto their server and this is carried out via a simple browse option which will allow the user to locate any file accessible locally or visible on the user's in-house network (Figure 3).

One big advantage of this collaboration now comes into play, and that is the availability of a multitude of file converters from Galactic Industries so that the spectral file to be uploaded can remain in the original spectrometer software's native format. A list of the
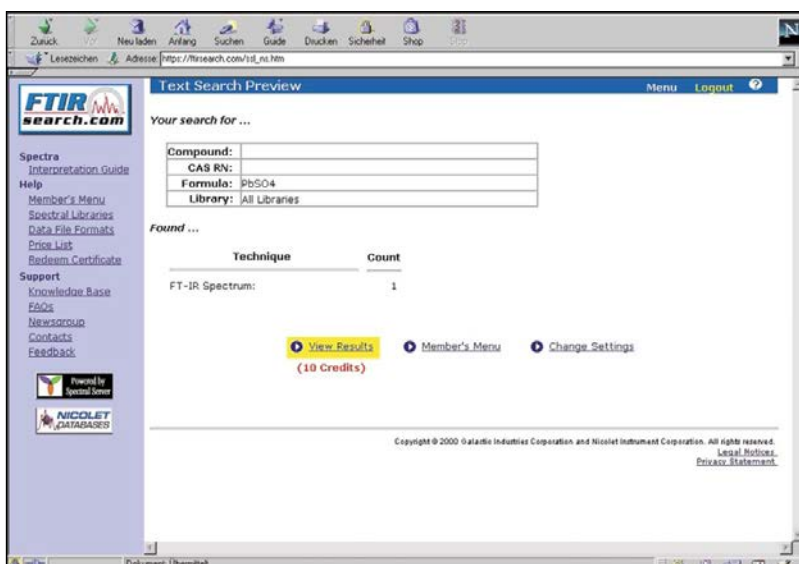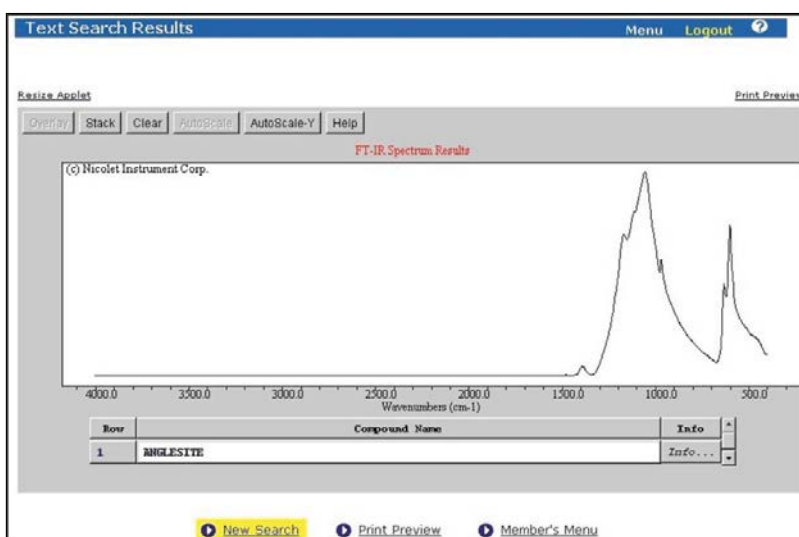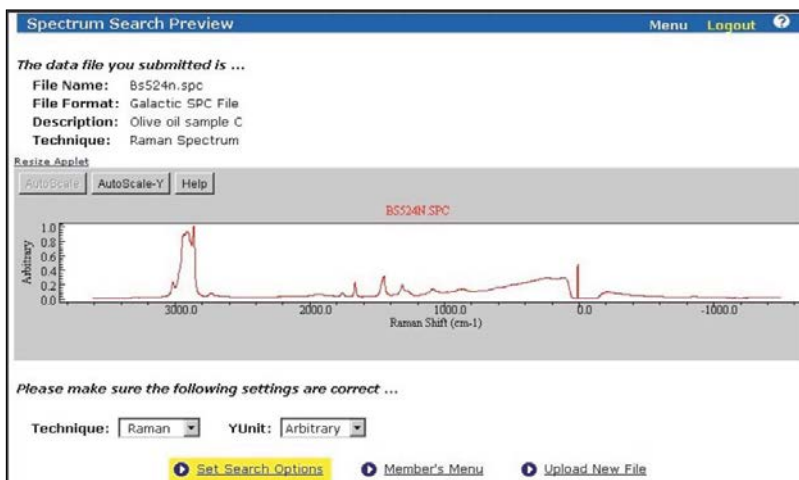
**Figure 1.**



**Figure 2.**
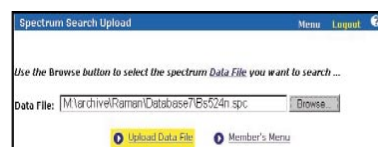


**Figure 4.**



**Figure 3.**

ried out!). This done, the next rather useful view the user gets is a preview to check the file has been imported accurately and that the axes have been correctly identified (Figure 4). This can be corrected at this stage.

If you are happy with the preview (our example is an adulterated olive oil sample measured by FT-Raman spectroscopy, both sides of the laser line giving Stokes and anti-Stokes data) then the next step is to set up the search options. In the advanced mode more options are available using different search algorithms which are also explained if somewhat hidden away in the "help members menu" section. This includes substantial assistance for those not familiar with the various full spectral search algorithms. The help explains not only exactly what happens mathematically during the spectral search but also advice on when to use which particular algorithm.

If you have reached this stage you will now realise that there is in reality no difference between the simple and advanced search entry options as all roads lead to Rome and the advanced options are also presented if you had started with the simple spectral search button! (Figure 5).

Figure 5, which shows a rather badly water compensated GC/IR PCB spectrum, also shows one of the drawbacks of the current system for infrared spectroscopists in that the IR databases can only be opted for in pre-determined blocks (forensic, industry specific, polymer, Sigma/Aldrich condensed phase or finally vapour phase). Raman spectroscopists are able to select specific databases—presumably because of the lower number of options.

The database search software is Galactic's Spectral Server which also powers their free spectral search site at: http://spectra.galactic.com/spconline/ where more than 6000 spectra of various spectroscopy types are available for searching. The functionality of this free service is much more limited than the version at http://ftirsearch.com.

And so to the results. Our search for the contaminated olive oil using the least squares search option yielded olive oil in third place which is a reasonable result considering the lack of any sample preparation and the presence of mild fluorescence and bands from the
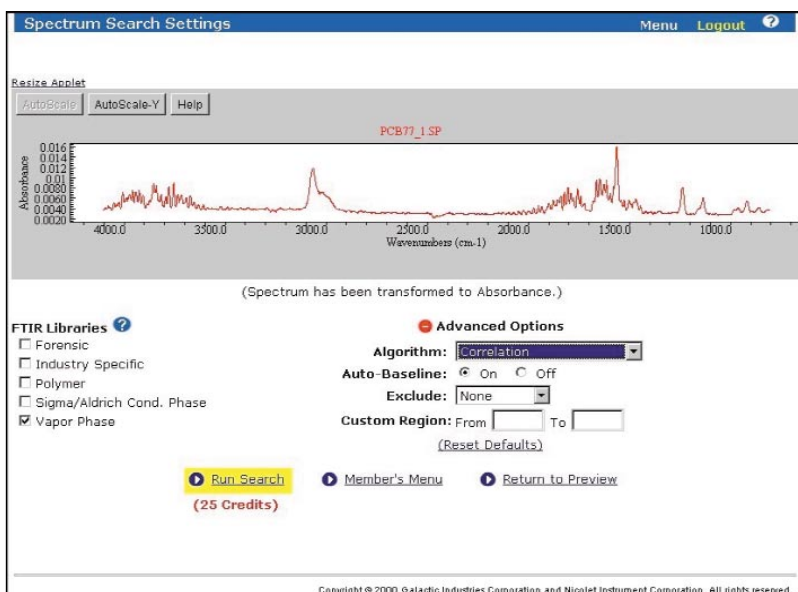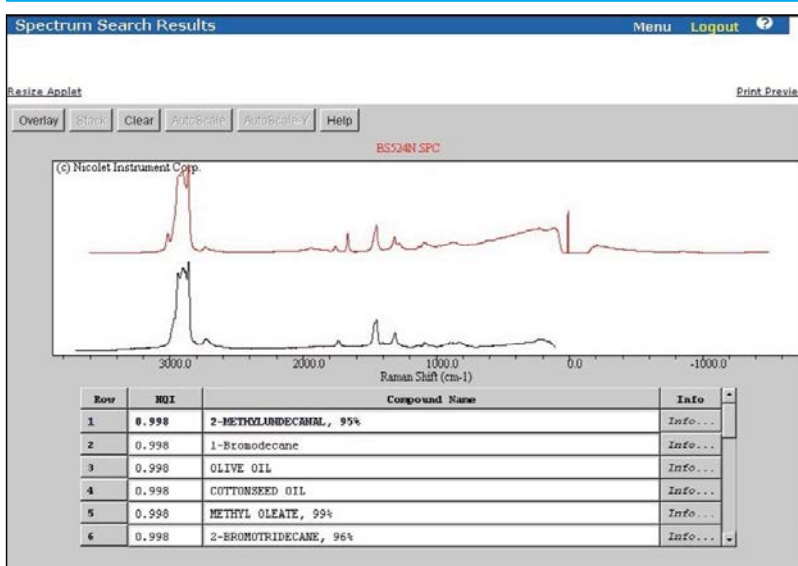
formats currently supported is available on the web site. In this on-line implementation the data format converter is somewhat cleverer than the stand-alone version with which I am acquainted, in that it automatically recognises the file format which it is being presented (at least for the limited testing I have car-
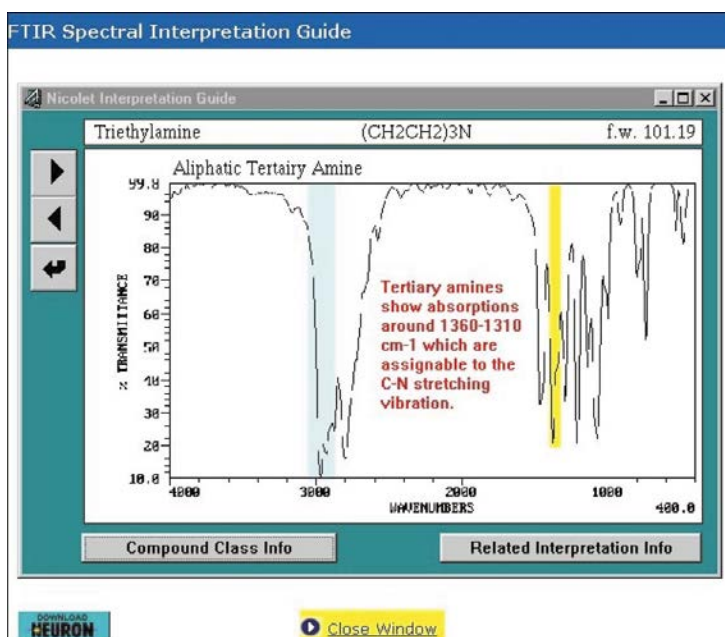
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**Figure 5.**



**Figure 6.**



**Figure 7.**

glass sample container which are clearly visible in the spectrum (Figure 6).

By playing with the search algorithm used I only succeeded in placing the olive oil result down to 4th place in the hit list although I did alter the hits which appeared above it!

The spectral range used for the search depends on two factors, one is the actual range of data stored in the libraries and the second is whether any area of the spectrum has been deliberately "left out" of the search by use of the advanced options.

# Spectral interpretation guide

Having had you install the Neuron plug-in at the beginning of the article it is only right to spend some time on the feature for which it is required. The Nicolet Spectral Interpretation Guide is available free to registered members and so will continue to be available after you have used up your test credits from the certificate. This simple guide aids the interpretation of infrared spectra by helping to identify the prominent spectral features of particular classes of compounds. The example shown in Figure 7 is for tertiary amines and by clicking on the blue highlighted areas the explanation appears.

The poor resolution is unfortunately one problem with this guide as is the none-scalable nature of the window itself. This is mainly due to the providers investing most of their energy in getting the spectral searching system up-and-running. Hopefully if it receives significant acclaim or accesses, the system developers might be persuaded to invest a small amount of time re-vamping what could well be a popular feature, especially amongst academic institutions, drawing people to the site.

# Conclusions

Considering the short amount of time the system has been up and running, the basic features promised function well. The unique ability to read so many formats makes for greater ease of access and the system managers decision that, although much of the system runs through the Java language, to avoid unnecessary flamboyance means that access times are good and the system stable. Galactic and Nicolet should be congratulated on their addition to the spectroscopist's arsenal of analytical tools.

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